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To aid in the development of boron-enhanced fluoro-nitramino explosives, the kinetics of individual reactions from those systems are investigated over wide temperature ranges. For BO + O_2 → BO_2 + O the measurements agree with earlier observation in the 400 - 1000 K range. No reaction could be observed between BO and CO_2 from 780 to 1200 K, indicating k less than $1x10^{-15}$ $cm^3molecule^{-1}s^{-1}$. For BO + N_2O → BO_2 + N_2 k(305-920 K) = $3x10^{-13}exp(-1310\ K/T)$ $cm^3molecule^{-1}s^{-1}$ was obtained.

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PROGRESS

Our goals are:

(i) to make accurate measurements, over wide temperature ranges, of rate coefficients for boron combustion in C/H/N/O/F environments, of importance to the development of new underwater explosives, and

(ii) to use the measurements to obtain a further understanding, to allow predictions for additional reactions occurring with such explosives.

The measurements are made by laser-induced fluorescence, LIF, in high temperature reactors. Our efforts in this first year have concentrated on the development of methods for introducing BO in HTFFRs (high-temperature fast-flow reactors). A large number of methods were investigated. The best are: i) those by which B atoms are produced in a microwave discharge, followed by reaction with O atoms or SO_2, and ii) those where $LiBO_2$, HBO_2, or B_2O_3 are vaporized and passed through a microwave discharge. However, all led to rate coefficients somewhat decreasing with residence time. This appears to be due to rapid wall dimerization of BO. Nonetheless, we obtained measurements on $BO + O_2 \rightarrow BO_2 + O$ between 400 and 1000 K. These are in essential agreement with earlier measurements[1] on this reaction of $k(300\text{-}1000\ K) = 7.0 \times 10^{-12} \exp(255\ K/T)\ cm^3 molecule^{-1} s^{-1}$. There a reactor fashioned after our real-time MHTP (metals high-temperature photochemistry) apparatus was used. Since further BO reactions show the same problem, we will use the HTFFR to determine approximate rate coefficients and make accurate measurements in the MHTP apparatus, which provides a wall-less reaction environment. The HTFFR equipment is still required for measurements from about 1000 to 1800 K, where the BO production method developed[1] for the photo-initiated reaction can not be used.

Two sets of such approximate measurements have already been made. The first of these is for the $BO + CO_2 \rightarrow BO_2 + CO$ reaction. While at room temperature a slow pressure-dependent reaction was observed, from 780 to 1200 K (the highest temperature explored thus far) no reaction was found. This indicates rate coefficient values less than about $1 \times 10^{-15}\ cm^3\ molecule^{-1}\ s^{-1}$. This is four orders of magnitude

lower than obtained for the BO + O_2 reaction. Even more importantly, it is two to four orders of magnitude lower than the guestimated values in the current models.[2-4] While the BO + CO_2 reaction and its reverse are considered to be highly sensitive for boron combustion in hydrocarbon systems,[2,3] they are not regarded so for the envisioned fluoro-nitramino based explosives.[4] However, such a large difference is important for those as well, once again illustrating the importance of measurements for the development of realistic models.

The measurements on the BO + $N_2O \rightarrow BO_2 + N_2$ reaction have yielded $k(305\text{-}920\ K) = 3\times10^{-13} \exp(-1310\ K/T)\ cm^3\ molecule^{-1}s^{-1}$.

PLANS

Preparations for work on the BO + HCl and BF_3 reactions have started. Once those measurements have been made below 1200 K, work on this reaction and the O_2 and CO_2 reaction above 1200 K in the HTFFR will start. (The N_2O study is restricted to the 920 K limit because of thermal instability.) For such higher temperature work BO LIF measurements will be made at shorter wavelengths, to reduce potential wall radiation interference.

We also plan to test the compatibility of our reactor materials with HF at high temperatures for measurements with that crucial reactant. For the study of the other boron species of ONR interest, BO_2 and BF, no similar problems as encountered with BO are expected and the HTFFR technique will, at least initially, be used for their study. Additionally to the above two high-temperature techniques, where laser-induced fluorescence is used for monitoring of the boron species, our HTFFR-mass spectrometer will be used for product identification. Especially product OBF detection would be important.

PARTICIPANTS AND CONTACTS

The experimental work has been performed by G.T. Dalakos with help from D.P. Belyung. In addition to these two students, W.F. Flaherty, our group technician, has participated.

We thank R.A. Yetter of Princeton University and M. Soto and L. Pasternack of the Naval Research Laboratory for helpful discussions on the kinetics aspects of the Navy program in underwater explosives.

PUBLICATIONS AND AWARDS

None this year.

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